Parametric Equation of State and Correlations in Supercritical Water and Krypton: a Comparison.

M. Bonetti^{C,S} Service de Physique de l'Etat CondensÈ CEA de Saclay F-91191 Gif-sur-Yvette, France

P. Calmettes
Laboratoire LÈon Brillouin
CEA de Saclay
F-91191 Gif-sur-Yvette, France

C. Bervillier Service de Physique ThÈorique CEA de Saclay F-91191 Gif-sur-Yvette, France

Understanding the behavior of supercritical fluids requires an accurate description of the cross-over region between the critical and the regular behavior. Small-angle neutron scattering (SANS) experiments performed at critical and off-critical densities allow this thermodynamic region to be probed and information about the scaling function and the corrections to scaling to be obtained. We present SANS spectra measured in the supercritical region for heavy water [1] and krypton [2]. The main difference between these two systems is that orientation correlations are absent in krypton. The SANS spectra were recorded for wave number transfers up to $0.36 \approx^{-1}$. The studied range of reduced density, $(\rho \tilde{n} \rho_c)/\rho_c$, and temperature, $(T\tilde{n}T_c)/T_c$, were [-0.176, 0.233] and [1.8 10^{-3} , 8.5 10^{-3}] for D₂O, and [-0.240, 0.224] and [1.0 10^{-3} , 9.5 10^{-2}] for krypton, respectively. ρ and T are the density and temperature and ρ_c and T_c their critical values, respectively.

The spectra are analysed using a parametric equation of state with appropriate corrections to scaling that include odd terms to account for the asymmetric behavior of the system. It will be shown that the critical contribution can be accurately described by the scaling function of Bray and an additional multiplicative term that describes the short-range correlations.

- [1] M. Bonetti, P. Calmettes, and C. Bervillier, J. Chem. Phys. 115, 4660 (2001).
- [2] M. Bonetti, P. Calmettes, and C. Bervillier, in preparation.